Antiphase Stripe Order as the Origin of Electron Pockets Observed in 1/8-Hole-Doped Cuprates

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Recent quantum oscillation measurements on underdoped cuprates are shown to be consistent with the predictions of a mean field theory of the 1/8 magnetic antiphase stripe order proposed to occur in high-T_c cuprates. In particular, for intermediate values of the stripe order parameter, the magneto-transport is found to be dominated by an *electron* pocket.

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The interplay between magnetism and superconductivity is an enduring theme in the physics of high-temperature copper-oxide superconductivity. These superconductors are created by doping antiferromagnetic insulating "parent compounds", and a wide variety of magnetic phenomena have been observed in both doped and undoped cuprates. One of the most interesting magnetic states proposed for the hole-doped cuprates is the 1/8 antiphase stripe state. This state has the spin and charge pattern sketched in Fig. 1: a modulation of the charge density which has the translation symmetry of the lattice along one direction ($\hat{y}$) and a four unit cell repeat distance along the orthogonal direction ($\hat{x}$). The basic spin pattern is a two-sublattice antiferromagnet, but the lines of minimum charge density are taken to be antiphase domain boundaries for the magnetization. This state was first predicted in Hartree-Fock calculations of Zaanen and Gunnarsson [1], Machida [2], and Littlewood and Inui [3]. It was later discussed extensively by Kivelson and collaborators (for a review, see Ref. 4).

A non-superconducting stripe phase has been unambiguously established as the ground state of $La_{1.875}Ba_{0.125}CuO_{4-\delta}$ [5] in which the hole density per unit cell is 1/8. A magnetically ordered state (believed to be a stripe phase) can be induced by applying a magnetic field to the superconducting state of $La_{2-x}Sr_xCuO_{4-\delta}$ (LSCO) [6] for a range of x around 1/8. Various anomalies associated with 1/8 doping have been seen clearly in other La_2CuO_4-derived materials [7, 8, 9], suggesting that a stripe phase, although perhaps not the ground state, is very nearby in free energy and influences measured properties, for example by competing with the superconducting state. However, the relevance of stripe phases to other members of the high-T_c family, in particular the $YBa_2Cu_3O_{7-\delta}$ (YBCO) family of superconductors, has been less clear. Magnetic fluctuations are observed in underdoped YBCO, but in the best samples, zero field magnetic order is apparently observed only in very underdoped compounds in the region where superconductivity has already vanished [10]. Transport [11, 12] and magneto-optical [13] data have been argued to be indications of density wave or stripe order in moderately-underdoped YBCO materials, and the "$60K$ T_c plateau" has also been suggested [14] to arise from 1/8 effects similar to those seen in LSCO. While these experiments have been suggestive, definitive proof of magnetic ordering has been lacking.

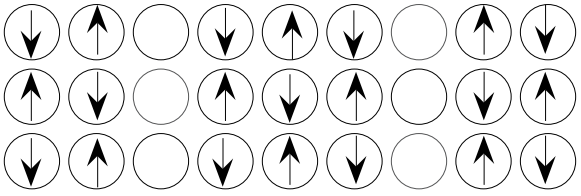

FIG. 1: Sketch of the magnetic and charge density in the 1/8 stripe state proposed for cuprate superconductors. Circles represent copper ions with their surrounding oxygens, arrows denote the copper spins, and empty circles indicate the "charge stripe" (antiphase domain wall).

Recently, a very remarkable series of magneto-transport experiments have transformed the situation. In ultra-pure samples of ortho-II $YBa_2Cu_3O_{6.5}$ [15] and $YBa_2Cu_4O_8$ [16, 17], quantum oscillations have been observed at fields above about $50T$. The measured oscillation frequencies suggest that the signal arises from small Fermi surface "pockets" such as might be produced by density wave ordering [15, 16, 17, 18]. Very recently, LeBoeuf *et al.* [19] have found that the temperature below which the high-field Hall coefficient becomes negative peaks at a doping of 1/8, providing strong evidence that the quantum oscillations arise from a Fermi surface reconstruction caused by "1/8" type ordering. However, the sign of the measured Hall conductance suggests that the transport arises from *electron* pockets [19], whereas the prevailing consensus is that hole pockets are expected: in particular, a simple two-sublattice ordering pattern does not yield robust electron pockets [18] while a large-amplitude stripe ordering would be expected to lead to effectively one dimensional transport characterized by open Fermi surfaces which would not give rise to magneto-oscillations.

In this communication we present a theoretical investigation of the Fermi surface and oscillation frequency implied by a stripe ordering pattern such as that sketched in Fig. 1. Generically, complicated Fermi surfaces occur involving open orbits, hole pockets and electron pockets. However we find that in some intermediate parameter regimes, the periodic potential associated with the stripe state can produce a Fermi surface consisting of a set of open (quasi one dimensional) bands, along with a single, simple electron pocket. The open orbits will make no contribution to the magneto-oscillations, while the electron pocket exhibits properties which are are in qualitative agreement with the magneto-oscillation data. We therefore argue that the recent magneto-transport data support the idea that stripe phases (competing with superconductivity, and most probably field-induced) are generic to hole-doped cuprates.

We consider the canonical tight-binding model of electrons hopping on a square lattice which is believed to describe the Fermi surface of the cuprates:

$$\begin{aligned} \varepsilon_k &= -2t\left(\cos k_x + \cos k_y\right) + 4t' \cos k_x \cos k_y \\ &\quad -2t''\left(\cos 2k_x + \cos 2k_y\right) - \mu \end{aligned} \tag{1}$$

where following Ref. 20 we choose $t = 0.38eV$, $t' = 0.32t = 0.122eV$ and $t'' = 0.5t' = 0.061eV$, noting that μ is the chemical potential. We express momenta in π/a units, with a the lattice parameter of the underlying square lattice.

We assume that electrons moving in this band structure are scattered by potentials with the periodicity of the stripe order. As can be seen from Fig. 1, the stripe state has a unit cell containing 8 sites of the underlying lattice. Fourier transforming the spins, we obtain a potential V_n connecting the state $\mathbf{k}$ with those at $\mathbf{k} \pm n\mathbf{Q}$ with $\mathbf{Q} = (3\pi/4, \pi)$. We expect that the term V_1 will be the dominant spin-derived scattering term, with a weaker third harmonic V_3 at $3\mathbf{Q}_\pm$. There will be a charge component V_2 at $2\mathbf{Q}_\pm$ with a weaker second harmonic at $4\mathbf{Q}_\pm$. We have found that the influence of V_3 and V_4 on our results is minor; these terms will be neglected here. Relabeling the spin potential V_1 as V and the charge potential V_2 as V_c, the resulting Hamiltonian may be written as an 8×8 matrix for $\mathbf{k}$ in the first Brillouin zone of the ordered state

$$H = \begin{pmatrix} \varepsilon_k & V_c & 0 & V_c & 0 & V & V & 0 \\ V_c & \varepsilon_{k+(\frac{1}{2},0)} & V_c & 0 & 0 & 0 & V & V \\ 0 & V_c & \varepsilon_{k+(1,0)} & V_c & V & 0 & 0 & V \\ V_c & 0 & V_c & \varepsilon_{k+(\frac{3}{2},0)} & V & V & 0 & 0 \\ 0 & 0 & V & V & \varepsilon_{k+(\frac{1}{4},1)} & V_c & 0 & V_c \\ V & 0 & 0 & V & V_c & \varepsilon_{k+(\frac{3}{4},1)} & V_c & 0 \\ V & V & 0 & 0 & 0 & V_c & \varepsilon_{k+(\frac{5}{4},1)} & V_c \\ 0 & V & V & 0 & V_c & 0 & V_c & \varepsilon_{k+(\frac{7}{4},1)} \end{pmatrix} \tag{2}$$

We have diagonalized this matrix and determined the Fermi surface for various dopings and V_n (note that the chemical potential has to be adjusted for each set of V_n to preserve the doping). We find that the Fermi surfaces are most easily visualized if the results are plotted not in the reduced Brillouin zone, but in a quadrant of the full square lattice zone $(0 < k_x < 1), (0 < k_y < 1)$.

To understand the results, it is useful to examine first the non-ordered ($V = V_c = 0$) case. Fig. 2a shows the Fermi surface from Eq. 1 at 1/8 hole doping. The Fermi surface is a large hole surface centered at the point $(1, 1)$. Fig. 2b shows this Fermi surface, along with the surface translated by multiples of $\mathbf{Q}_\pm$. The result is a highly complicated set of bands. The key feature, however, is the nearly flat segments. These arise from the portions of the Fermi surface which approach the zone boundaries $k_x = 1/k_y = 1$. We shall see that the scattering potential implied by the stripe order reconnects these into an electron pocket, which exists over a wide range of parameter values.

The four panels of Fig. 3 shows the effect of the stripe order. Panel a shows the effect of a weak spin potential with no charge potential. The resulting Fermi surface is reconstructed and begins to reveal the one dimensional structure associated with motion along the stripe direction. The electron pocket has also emerged, although its size is considerably larger than that observed in Ref. 15.

Panel b shows the Fermi surfaces implied by the stronger coupling $V = 0.2eV$ (with $V_c = 0$). The increase in V shrinks the electron pocket and separates it from the one dimensional band. In addition, the "zig-zag" band has pinched off, leading to hole pockets. Reducing the hole doping to 1/10 or moderately increasing V causes these hole pockets to decrease and ultimately disappear, leaving only electron pockets. For yet larger V, the electron pockets vanish and only the quasi one dimensional bands remain.

Panels c and d explore the effect of adding a potential

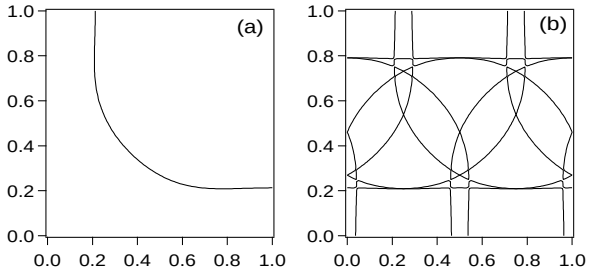

FIG. 2: (a) Fermi surface from Eq. 1, corresponding to a hole density of 1/8, plotted in the first quadrant of the Brillouin zone of the underlying square lattice (note that π/a momentum space units are used in all figures). (b) Fermi surface in (a) plus its images under translation by the stripe order (multiples of $\mathbf{Q}_{\pm}$), equivalent to Eq. 2 with $V = V_c = 0$.

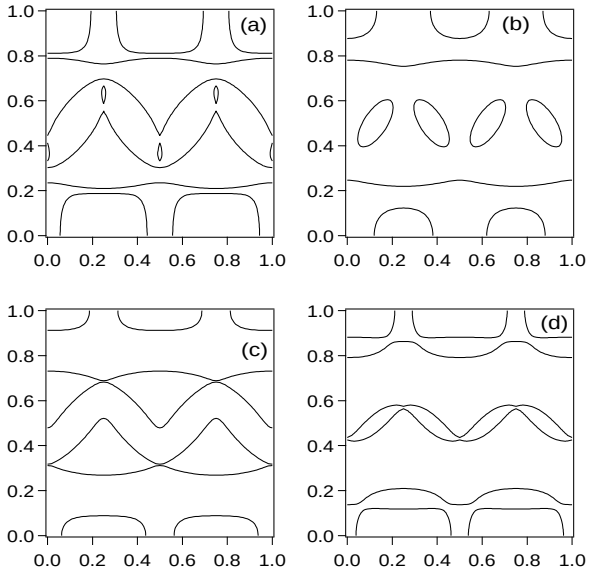

FIG. 3: Fermi surfaces from Eq. 2 with a hole doping of 1/8 plotted in the first quadrant of the Brillouin zone of the underlying square lattice: (a) $V = 0.1eV$, $V_c = 0$, (b) $V = 0.2eV$, $V_c = 0$, (c) $V = 0.2eV$, $V_c = 0.15eV$, and (d) $V = 0.2eV$, $V_c = -0.2eV$.

due to the charge order. Fourier transformation of the standard stripe ordering pattern implies $V_c > 0$ as may be understood from the lower *electron* density on the charge stripe row, but for completeness we show both signs. In both cases the effect of V_c is to reconnect the hole pockets into one dimensional bands; the $V_c < 0$ case tends to eliminate them more rapidly than does $V_c > 0$.

One question which arises is the relative effects of magnetic and charge order. To investigate this point, we have re-computed the Fermi surface for the case $V = 0$ with varying V_c (i.e., assuming that the magnetic order has a negligible effect on the electron dynamics). A representative Fermi surface is shown in Fig. 4a. We see that in the

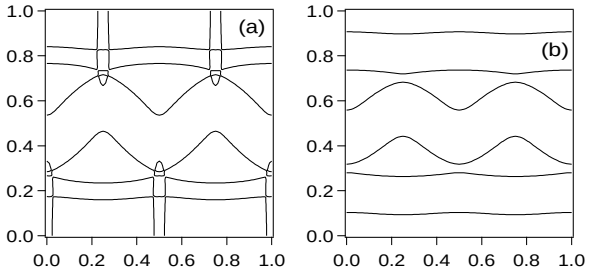

FIG. 4: Fermi surface from Eq. 2 with $V = 0$ and (a) $V_c = 0.1eV$ and (b) $V_c = 0.2eV$, for 1/8 hole doping, plotted in the first quadrant of the Brillouin zone of the underlying square lattice.

absence of spin order, the pockets have a very extreme aspect ratio. As the potential is made stronger, the aspect ratio of the pocket increases until it collapses into a single line and vanishes (Fig. 4b). And in this purely charge case, the pocket is a hole pocket. We conclude that the potential produced by spin ordering plays the essential role in the formation of the observed electron pocket.

We next examine in more detail the pockets implied by our calculations. Within the model, the size of the electron pockets depends strongly on V; the value of V may therefore be adjusted to produce any area desired at a given doping. Since there are 8 magnetic zones per square lattice zone, and there is 1 electron pocket per magnetic zone, a pocket with size 7.6% of the area of the first quadrant of the square lattice Brillouin zone, as seen in Ref. 15, corresponds to an occupation factor of 0.038 electrons per copper atom (noting that the magnetic state retains a Kramers degeneracy).

The electron pocket, centered at the magnetic zone boundary, $(1/4, 0)$, has a cyclotron mass which varies from 0.5 to 1.0 for the various cases shown in Fig. 3. The hole pocket in Fig. 3b has a lighter cyclotron mass of 0.3. Therefore, if such a hole pocket existed, it would be very apparent in any magneto-oscillation measurement. The measured cyclotron mass is $1.9m_e$ [15]. We suggest that the difference between the calculated and measured masses is due in large part to the renormalization of band theory inferred from other measurements. For example, the nodal velocity measured in angle-resolved photoemission experiments is about $1.6eV\mathring{A}$ [21], which is reduced from the calculated band velocity of $3.8eV\mathring{A}$ from Eq. 1 by a factor of 2.4. Such a renormalization would imply a bare cyclotron mass of 0.8, which is within the range of the values we find for the electron pocket.

In summary, we have shown that at intermediate coupling, a periodic potential such as would be produced by a magnetic antiphase domain "stripe" structure produces electron pockets which are consistent with experiment, if the energy scales are renormalized from band theory by a factor similar to that observed from angle-resolved

photoemission experiments. The results are sensitive to the details of the scattering potential: in particular, for stronger potentials $V \gtrsim 0.3eV$, only open orbits associated with one dimensional transport along the stripe direction exist, whereas for a range of combinations of spin and charge potentials, both electron and hole pockets are found, though the latter exist for a much narrower range of parameters than the former. We emphasize, though, the generic feature of our results, namely that the spin potential associated with antiphase stripe order produces robust electron pockets in hole-doped high-T_c superconductors. These results confirm the interpretation of Ref. [15] that the quantum oscillations imply the existence of a density wave state at high magnetic fields in the YBCO cuprates, and indeed confirm the identification of the state as the 1/8 magnetic antiphase stripe state discussed by many workers. However, we note that our results (and, more fundamentally, the identification of electron pockets) imply that the ordering is not strong enough to confine the electron motion completely to one dimensional paths. Our findings suggest several further directions for research. X-ray or elastic neutron scattering experiments should be performed at high fields to confirm this identification. Further, as noted by Ando *et al.* [12], stripes in the YBCO materials are expected to be aligned along the chain direction; thus in single-domain samples, the stripe domains may all be aligned, leading to an increase in the anisotropy. Optical and magneto-optical experiments may reveal evidence of the excitation gap implied by the stripe order. A future paper will present a more comprehensive theoretical investigation, including the effects of bilayer coupling and oxygen ordering, as well as computing in detail the magneto-transport and magneto-optical properties of the various states.

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